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by Erwin Fehlberg

George C. Marshall Space Flight Center
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By

Erwin Fehlberg

SECTION I. INTRODUCTION

1. The methods for the numerical integration of initial value problems in ordinary differential equations can be divided into two classes--multistep methods and one-step methods.

2. Multistep methods were developed as early as the nineteenth century, mainly for astronomical problems. As their name indicates, these methods use the information from several backward (or also forward) computation steps in calculating the solution for the current step. Multistep methods (such as the ADAMS, GAUSS, COWELL, etc. methods) are very useful in problems for which the numerical integration can be performed with a constant step size. Since many such problems are encountered in astronomy, it is quite natural that astronomers have developed a number of powerful multistep methods. Moreover, since these multistep methods can be extended to any order of accuracy (simply by adding higher-order difference terms to the formulas) and since, in general, they require only one or two evaluations of the differential equations per step, they seem to represent a rather rapid and economical integration procedure.

3. However, multistep methods do have certain inconveniences and disadvantages:

A. They are not self-starting but require a special starting procedure.

B. Halving the step size during the computation requires time-consuming iterations to build a new difference scheme.

C. The truncation error for multistep methods is larger than for one-step methods of corresponding order. Multistep methods therefore require a smaller step size than corresponding one-step methods.

D. The classical multistep methods are, for stability reasons, of only a mediocre order of accuracy, considering the number of steps involved. Although a k-step formula for the solution of a first-order differential equation contains $2k+1$ constants, there exists no numerically stable k-step formula of an order exceeding $k+1$ (for odd k) or $k+2$ (for even k). This means that the stability requirement reduces the possible order $2k$ of such a k-step formula by $k-1$ or $k-2$, respectively.

4. Only recently, W. B. GRAGG and H. J. STETTER [14] have succeeded in eliminating the stability restrictions of the classical multistep methods by introducing into the formulas one extra non-step point. Such modified multistep formulas have been published by J. C. BUTCHER [8]. His paper contains numerically stable k-step predictor-corrector formulas of order $2k+1$ for $k \leq 6$. Since our paper deals with one-step methods, we shall consider one of J. C. BUTCHER's new multistep formulas in Appendix C for comparison only.

5. In one-step methods, no information obtained from previously computed steps is required. Most one-step methods are of the RUNGE-KUTTA type. In RUNGE-KUTTA formulas the necessary information is obtained by repeated evaluation of the differential equation at intermediate points somewhere between the initial and the end point of the current step.

Since the standard RUNGE-KUTTA formulas are of fourth-order accuracy only--the truncation errors being of the fifth order of the step size--several extensions of these formulas to higher-order accuracy have been achieved in the last decade. We mention in this respect the work of A. HUŤA [15], [16], J. C. BUTCHER [1], [2], [3], [6], and E. B. SHANKS [18], [19]. The last author has derived the most accurate RUNGE-KUTTA formula to date--an eighth-order formula based on 12 evaluations per step.

6. Like all one-step methods, the RUNGE-KUTTA method is self-starting and the integration step size can be changed at any time and can immediately be accommodated to the local conditions of the problem under consideration. In this respect, RUNGE-KUTTA methods are well-suited to problems that require frequent changes in the step size. However, RUNGE-KUTTA methods also have certain disadvantages. They are time-consuming, since they require a relatively large number of evaluations per step of the differential equations. Moreover, no economical method of step-size control seems to exist for RUNGE-KUTTA formulas. Apart from somewhat doubtful rule-of-thumb control procedures, there exists only L. F. RICHARDSON's well-known method of the deferred approach to the limit. This method is quite reliable, but it doubles the computational effort merely for the benefit of step-size control.

7. This paper will describe some one-step methods that the author has developed. They are essentially a combination of power series expansions and RUNGE-KUTTA methods. When applicable, our formulas have definite advantages compared with standard RUNGE-KUTTA formulas: they yield any order of accuracy one might desire; they require only very few evaluations of the differential equations; they include a very simple and economical method of step-size control. We shall describe these new RUNGE-KUTTA methods in detail in Section III.

8. In Section IV we shall derive the equations of motion of the restricted problem of four bodies. Since this problem is of some practical interest in astronautics, in Sections V and VI we shall apply our new RUNGE-KUTTA procedure to this problem as well as to the restricted problem of three bodies.

9. For comparison we shall report, in the appendices, our experience with some new methods developed by other authors. These appendices will give brief descriptions and applications of the following methods:

   A. The explicit RUNGE-KUTTA formulas of E. B. SHANKS (Appendix A).

   B. The implicit RUNGE-KUTTA formulas of J. C. BUTCHER (Appendix B).

   C. The modified multistep method of J. C. BUTCHER (Appendix C).

10. A short abstract of a part of this paper was presented at the Congress of the International Federation of Information Processing (IFIP) in New York in May 1965 [13]. This joint presentation, by S. FILIPPI and the author, also included work by the authors on the LIE series method. Dr. FILIPPI intends, at a later date, to publish the results of his LIE series investigations as a NASA Technical Note.

SECTION II. POWER SERIES EXPANSION METHOD

11. The integration procedures that we shall describe in this and the following section are based on a power series expansion for the solution of the differential equations under consideration. Such a power series expansion requires a repeated total differentiation of the differential equations with respect to the independent variable in order to obtain the coefficients of the power series expansion.

In the past, the repeated total differentiation of a differential equation was considered unfeasible, since, with increasing order, the derivatives become rather unwieldy expressions. Today, with the advent of fast electronic computers, such a procedure no longer seems necessarily unfeasible. It is well-known that in the last few years considerable progress has been made in automatic formula differentiation by computers. Apart from a straightforward differentiation of the differential equations, a great number of differential equations can be differentiated in a rather simple way after transforming them--by introducing auxiliary functions--into algebraic differential equations of the second degree. For special differential equations the procedure has been outlined in earlier papers by J. F. STEFFENSEN [20], E. RABE [17], and the author [10]. The procedure is based on the fact that the consecutive derivatives of a second-degree system of differential equations can be conveniently obtained on a computer by recurrence formulas.

12. The procedure is best illustrated by a simple example. Let us consider the differential equation

$$\frac{dx}{dt} = e^{-x} \tag{1}$$

We introduce the auxiliary function

$$e^{-x} = u \tag{2}$$

and obtain from (1) and (2) a system of second-degree algebraic differential equations

$$\frac{dx}{dt} = u, \qquad \frac{du}{dt} = -u^2 \tag{3}$$

Substituting the power series expansions

$$x = \sum_{\nu=0} X_\nu (t-t_0)^\nu, \qquad u = \sum_{\nu=0} U_\nu (t-t_0)^\nu \tag{4}$$

into (3) and comparing coefficients for the terms with $(t-t_0)^n$ results in the following recurrence formulas for the coefficients in (4):

$$\left.\begin{aligned} (n+1)X_{n+1} &= U_n \\ (n+1)U_{n+1} &= -\sum_{\nu=0}^{n} U_\nu U_{n-\nu} \end{aligned}\right\} \quad (n = 0,\ 1,\ 2,\ \ldots) \tag{5}$$

Since the first coefficient X_0 is known from the initial value $x(t_0)$ for the step and the first coefficient U_0 can be obtained from (2), all following coefficients X_ν, U_ν ($\nu = 1,\ 2,\ 3,\ \ldots$) can easily be computed from the recurrence formulas (5)--a very convenient procedure for electronic computers.

13. It is quite obvious that the power series expansion method allows--in an extremely simple way--an automatic step-size control. Assuming that we truncate the expansion (4) for x after the term $X_n(t-t_0)^n$, the leading term of the truncation error of x can easily be found by extending the computation to the next

coefficient X_{n+1}. If the truncation error turns out to be too large or too small, the step size at Δt can immediately be adjusted in such a way that $|X_{n+1}(\Delta t)^{n+1}|$ remains within prescribed limits. For safety reasons it might sometimes be advisable to consider more than just one term of the truncation error. In contrast to RUNGE-KUTTA or multistep methods, no repetition of any computation is necessary if the step size fails to meet the requirements for the magnitude of the truncation error. We know of no other method that offers such easy step-size control.

14. Naturally, in our simple example No. 12, there is no real need to resort to the introduction of auxiliary functions, since a repeated differentiation of the differential equation (1) can be performed without difficulty. In Section IV we shall present more involved examples that do not allow a convenient repeated straightforward differentiation without the introduction of auxiliary functions.

SECTION III. RUNGE-KUTTA TRANSFORMATION TYPE FORMULAS

15. In two earlier papers [11],[12], the author presented RUNGE-KUTTA type formulas of high-order accuracy for the numerical integration of systems of first- and second-order differential equations. These formulas require a repeated total differentiation of the differential equations with respect to the independent variable. After m total derivatives are determined at the initial point $t = t_0$ of the step under consideration, using, for instance, the method of Section II, a transformation of the dependent variables of the differential equations is performed in such a way that, in the case of second-order differential equations, the first m+2 total derivatives of these transformed dependent variables become zero for $t = t_0$.

In the following we shall consider systems of second-order differential equations only, since these are the ones most frequently encountered in physics and mechanics. Moreover, our method is somewhat simpler in the case of second-order differential equations, because the number of RUNGE-KUTTA evaluations (including approximation of the truncation error) is reduced by 1 compared with the corresponding procedure for first-order differential equations.

16. Let x be the original dependent variable--for the sake of brevity we shall write our formulas for one second-order differential equation

$$\ddot{x} = f(t, x, \dot{x}) \tag{6}$$

only, although they hold in the same way for systems. Let x_T be the transformed dependent variable. Obviously the first m+2 total derivatives of x_T are zero for $t = t_0$ if we define

$$x_T = x - \sum_{\nu=1}^{m+2} X_\nu (t-t_o)^\nu \tag{7}$$

with the power series coefficients X_ν being defined as the ν-th derivatives of x at $t = t_o$, divided by the factorials $\nu!$.

From (7) it follows that

$$\dot{x}_T = \dot{x} - \sum_{\nu=1}^{m+2} \nu X_\nu (t-t_o)^{\nu-1} \tag{8}$$

$$\ddot{x}_T = \ddot{x} - \sum_{\nu=2}^{m+2} \nu(\nu-1) X_\nu (t-t_o)^{\nu-2}$$

$$\ddot{x}_T = f - \sum_{\nu=2}^{m+2} \nu(\nu-1) X_\nu (t-t_o)^{\nu-2} = f_T \tag{9}$$

Equation (9) represents the transformed differential equation

$$\ddot{x}_T = f_T(t, x_T, \dot{x}_T) \tag{10}$$

for which we derived, in papers [11], [12], RUNGE-KUTTA formulas of order m+4 as well as m+5.

These formulas require no more than four RUNGE-KUTTA evaluations of the differential equations,including the determination of the leading term of the truncation error for x_T.

The small number of evaluations required is strictly a consequence of the fact that the first m+2 derivatives of x_T are zero for $t=t_o$, since this behavior of the derivatives drastically reduces the number of equations of condition for the RUNGE-KUTTA coefficients.

Since we have given a rather detailed derivation of our RUNGE-KUTTA formulas in papers [11] and [12], we restrict ourselves here to stating these formulas and to explaining, with the help of a flow chart, how to program our formulas on an electronic computer.

17. First, we shall state the formulas derived in paper [11] for the case of second-order differential equations. The method described in this paper requires three RUNGE-KUTTA evaluations of (10) to obtain (m+4)-th-order formulas for x_T and $\dot{x}_T$ and one additional evaluation for an (m+5)-th-order formula for x_T, m always standing for the number of differentiations performed on the original differential equation (6) at the initial t-value $t = t_0$ of the current step. Using the traditional notation, the formulas of paper [11] read:

$$\begin{aligned} k_1 &= f_T(t_0 + h,\ x_0,\ 0)h \\ k_2 &= f_T(t_0 + \alpha_2 h,\ x_0 + \beta_0 k_1 h,\ 0 + \beta k_1)h \\ k_3 &= f_T(t_0 + h,\ x_0,\ 0 + \gamma k_1 + \delta k_2)h \\ k_4 &= f_T(t_0 + \alpha_4 h,\ x_0 + \varepsilon_0 k_1 h,\ 0 + \varepsilon k_1 + \zeta k_2 + \eta k_3)h \quad (h = \text{step size}) \end{aligned} \tag{11}$$

and

$$\left.\begin{aligned} x_T - x_0 &= C_{20} k_2 h + 0(h^{m+5}) \\ \hat{x}_T - x_0 &= (\hat{C}_{20} k_2 + \hat{C}_{30} k_3 + \hat{C}_{40} k_4)h + 0(h^{m+6}) \\ \dot{x}_T - 0 &= C_2 k_2 + C_3 k_3 + 0(h^{m+5}) \end{aligned}\right\} \tag{12}$$

From (7) and (8) there follow for the initial values of the current step:

$$x_T(t_0) = x(t_0)(=x_0), \quad \dot{x}_T(t_0) = 0 \tag{13}$$

These values (13) have already been inserted into (11).

The first two equations in (12) yield two values, x_T and $\hat{x}_T$, for $t = t_0 + h$ that differ in accuracy by one h-power. Therefore, their difference can be considered an approximation of the leading term of the truncation error of x_T.

The constants in formulas (11) and (12) are given by the following relatively simple expressions:

$$
\left.
\begin{aligned}
&\alpha_2 = \frac{m+2}{m+4}, \qquad \alpha_4 = \frac{m+1}{m+4} \\
&\beta_0 = \frac{2}{(m+4)^2}\left(\frac{m+2}{m+4}\right)^{m+1}, \qquad \epsilon_0 = \frac{3}{2}\cdot\frac{m-2}{(m+2)(m+4)^2}\left(\frac{m+1}{m+4}\right)^{m+1} \\
&\beta = \frac{1}{m+4}\left(\frac{m+2}{m+4}\right)^{m+1}, \qquad \gamma = -\frac{1}{m+2}, \qquad \delta = \frac{2}{m+2}\left(\frac{m+4}{m+2}\right)^{m+1} \\
&\epsilon = \frac{1}{2}\cdot\frac{m-5}{(m+2)(m+4)}\left(\frac{m+1}{m+4}\right)^{m+1}, \qquad \zeta = \frac{5}{4}\cdot\frac{1}{m+2}\left(\frac{m+1}{m+2}\right)^{m+1} \\
&\eta = -\frac{3}{4}\cdot\frac{1}{m+4}\left(\frac{m+1}{m+4}\right)^{m+1} \\
&C_{20} = \frac{1}{(m+2)(m+3)}\left(\frac{m+4}{m+2}\right)^{m+1}, \qquad C_2 = \frac{1}{2}\cdot\frac{m+4}{(m+2)(m+3)}\left(\frac{m+4}{m+2}\right)^{m+1} \\
&C_3 = \frac{1}{2}\cdot\frac{1}{m+3}, \qquad \hat{C}_{20} = \frac{3}{(m+2)(m+3)(m+5)}\left(\frac{m+4}{m+2}\right)^{m+1} \\
&\hat{C}_{30} = \frac{1}{3}\cdot\frac{1}{(m+3)(m+5)}, \qquad \hat{C}_{40} = \frac{2}{3}\cdot\frac{1}{(m+3)(m+5)}\left(\frac{m+4}{m+1}\right)^{m+1}
\end{aligned}
\right\} \qquad (14)
$$

It should be pointed out that the leading term of the truncation errors of x_T and $\dot{x}_T$ is not particularly small in our formulas. The situation is somewhat similar to that for the standard 4-th-order RUNGE-KUTTA formulas. In both methods, a part of the respective (m+5)-th-order or 5-th-order terms in the Taylor expansion for the solution is not covered at all. However, the extent

to which these leading terms of the truncation error are partially covered is very essential for the accuracy of such a method. A good coverage of these terms pays off by allowing a larger integration step size than in the case of a formula of the same order but with a larger truncation error.

18. In paper [12] we presented formulas with smaller truncation errors than those in paper [11]. In fact, in the formulas in paper [12], a parameter σ is still available, and for sufficiently small values of σ the absolute values of all members of the leading truncation error term, for x_T as well as for $\dot{x}_T$, can be made as small as desired. However, they cannot be made zero, since some of the weight coefficients of our formulas would become infinite for $\sigma \to 0$.

These more accurate formulas read as follows:

$$\left.\begin{aligned} k_1 &= f_T(t_0 + h,\ x_0,\ 0)h \\ k_2 &= f_T(t_0 + \alpha_2 h,\ x_0 + \beta_0 k_1 h,\ 0 + \beta k_1)h \\ k_3 &= f_T(t_0 + \alpha_3 h,\ x_0 + \gamma_0 k_1 h + \delta_0 k_2 h,\ 0 + \gamma k_1 + \delta k_2)h \\ k_4 &= f_T(t_0 + h,\ x_0,\ 0 + \epsilon k_1 + \zeta k_2 + \eta k_3)h \end{aligned}\right\} \qquad (15)$$

and

$$\left.\begin{aligned} x_T - x_0 &= (C_{20}k_2 + C_{30}k_3)h + 0(h^{m+5}) \\ \hat{x}_T - x_0 &= (\hat{C}_{20}k_2 + \hat{C}_{30}k_3 + \hat{C}_{40}k_4)h + 0(h^{m+6}) \\ \dot{x}_T - 0 &= C_2 k_2 + C_3 k_3 + C_4 k_4 + 0(h^{m+5}) \end{aligned}\right\} \qquad (16)$$

Again, the initial values (13) have already been inserted into (15).

The constants in (15) and (16) are no longer as simple as the expressions (14). Expressed as functions of the parameter σ, these coefficients read:

$$\alpha_2 = \frac{m+2}{m+5}(1-\sigma), \qquad \alpha_3 = \frac{1-\sigma}{1+(m+4)\sigma^2}$$

$$\beta_0 = \frac{1}{2}\cdot\frac{\alpha_2^{m+1}}{(m+5)^2}[3+(m+2)\sigma][1-(m+6)\sigma], \qquad \beta = \alpha_2^{m+1}\frac{1-\sigma}{m+5}$$

$$\gamma_0 = -\frac{1}{2}\cdot\frac{1}{m+2}\alpha_3^{m+1}\sigma\frac{1+(m+4)\sigma}{1+(m+4)\sigma^2}\left[2+m\sigma\frac{1+(m+4)\sigma}{1+(m+4)\sigma^2}\right]$$

$$\gamma = -\alpha_3^{m+1}\frac{1-\sigma}{m+2}\cdot\frac{2-(m+3)(m+4)\sigma^2}{[1+(m+4)\sigma^2]^2}$$

$$\delta_0 = \frac{3}{m+2}\left(\frac{\alpha_3}{\alpha_2}\right)^{m+1}\cdot\sigma(1-\sigma)\frac{1+(m+4)\sigma}{[1+(m+4)\sigma^2]^2}, \qquad \delta = \left(\frac{\alpha_3}{\alpha_2}\right)^{m+1}\cdot\frac{1-\sigma}{m+2}\cdot\frac{3-(m+2)(m+4)\sigma^2}{[1+(m+4)\sigma^2]^2}$$

$$\epsilon = -\frac{2}{m+2}\cdot\frac{1-\sigma}{1-2(m+4)\sigma-(m+2)(m+4)\sigma^2}$$

$$\xi = \frac{1}{\alpha_2^{m+1}}\cdot\frac{1}{m+2}\cdot\frac{1}{1-\sigma}\cdot\frac{[3+(m+2)\sigma][3-(2m+13)\sigma+3(m+4)\sigma^2+(m+2)(m+4)(m+6)\sigma^3]}{[3-(m+2)(m+4)\sigma^2][1-2(m+4)\sigma-(m+2)(m+4)\sigma^2]}$$

$$\eta = -\frac{1}{\alpha_3^{m+1}}\cdot\frac{\sigma}{1-\sigma}\cdot\frac{[3+(m+2)\sigma][1+(m+4)\sigma][1+(m+4)\sigma^2]}{[3-(m+2)(m+4)\sigma^2][1-2(m+4)\sigma-(m+2)(m+4)\sigma^2]}$$

$$C_{20} = \frac{1}{\alpha_2^{m+1}}\cdot\frac{m+5}{(m+2)(m+3)(m+4)}\cdot\frac{1}{1-\sigma}\cdot\frac{2-(m+4)\sigma-(m+2)(m+4)\sigma^2}{3-(m+2)(m+4)\sigma^2}$$

$$C_{30} = \frac{1}{\alpha_3^{m+1}}\cdot\frac{1}{(m+3)(m+4)}\cdot\frac{1}{1-\sigma}\cdot\frac{[1+(m+4)\sigma][1+(m+4)\sigma^2]}{3-(m+2)(m+4)\sigma^2}$$

$$C_2 = \frac{1}{\alpha_2^{m+1}}\cdot\frac{(m+5)^2}{(m+2)(m+3)(m+4)}\cdot\frac{1}{1-\sigma}\cdot\frac{2-(m+4)\sigma-(m+2)(m+4)\sigma^2}{[3-(m+2)(m+4)\sigma^2][3+(m+2)\sigma]}$$

$$C_3 = \frac{1}{\alpha_3^{m+1}}\cdot\frac{1}{(m+3)(m+4)}\cdot\frac{1}{\sigma(1-\sigma)}\cdot\frac{[1+(m+4)\sigma^2]^2}{3-(m+2)(m+4)\sigma^2}$$

$$C_4 = -\frac{1}{(m+3)(m+4)}\cdot\frac{1}{\sigma}\cdot\frac{1-(m+4)\sigma-(m+4)(3m+10)\sigma^2-(m+2)(m+4)^2\sigma^3}{[1+(m+4)\sigma][3+(m+2)\sigma]}$$

$$\hat{C}_{20} = \frac{2}{\alpha_2^{m+1}}\cdot\frac{m+5}{(m+2)(m+3)(m+4)}\cdot\frac{1}{1-\sigma}\cdot\frac{3-(m+5)\sigma-(m+2)(m+4)\sigma^2}{[3+(m+2)\sigma][3-(m+2)(m+4)\sigma^2]}$$

$$\hat{C}_{30} = \frac{2}{\alpha_3^{m+1}}\cdot\frac{1}{(m+3)(m+4)}\cdot\frac{1}{1-\sigma}\cdot\frac{[1+(m+4)\sigma^2]^2}{[1+(m+4)\sigma][3-(m+2)(m+4)\sigma^2]}$$

$$\hat{C}_{40} = -\frac{1}{(m+3)(m+4)}\cdot\frac{1-2(m+4)\sigma-(m+2)(m+4)\sigma^2}{[1+(m+4)\sigma][3+(m+2)\sigma]}$$

(17)

In paper [12] these coefficients (17) are tabulated to 24 digits--for m = 3 through m = 8. The parameter σ is always chosen in such a way that the absolute values for the critical coefficients C_3 and C_4 are about 1/2 or less. The advantage of these more accurate formulas over the earlier formulas (11), (12), (14) will show up clearly in the examples in Section VI.

19. It might be helpful to illustrate the application of our RUNGE-KUTTA procedure by means of a flow chart, as is customary for computer programs. As Figure 1, we present a flow chart for our more accurate formulas (15), (16). The flow chart for our earlier formulas (11), (12) is almost identical with the flow chart in Figure 1.

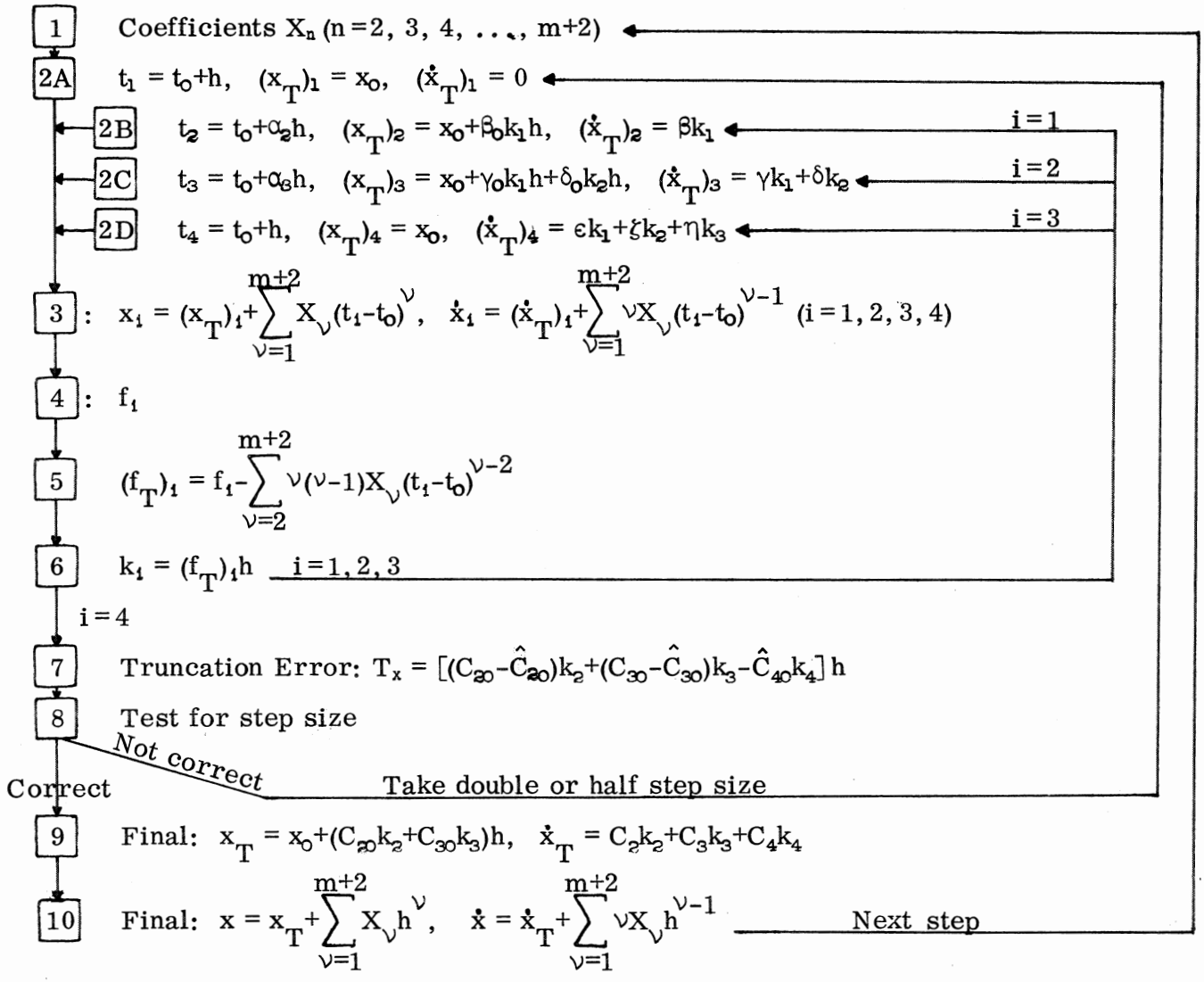

FIGURE 1. FLOW CHART

After having computed in [1] the power series coefficients $X_n (n=2, 3, \ldots, m+2)$ for the original differential equation (6) by the method indicated in Section II, then in [2] we introduce the proper arguments t, x_T, $\dot{x}_T$ for the RUNGE-KUTTA evaluations of the transformed differential equation (9). However, since we have to deal with the original differential equation (6) instead of (9) we proceed in [3] from x_T and $\dot{x}_T$ to x and $\dot{x}$ and evaluate in [4], for these arguments, the right-hand side of (6). In [5] we compute the right-hand side of (9), since our RUNGE-KUTTA procedure holds for the transformed differential equation (9) only. By multiplying by h we obtain in [6] the k_i-values (15) for the transformed differential equation (9). After having computer all four k_i-values $(i=1, 2, 3, 4)$, we determine in [7] the approximate truncation error for x_T. If necessary, the step size now has to be adjusted (by halving or doubling) in such a way that the truncation error remains within pre-set tolerances. After the step size has been checked and found to be satisfactory, the final values x_T and $\dot{x}_T$ for the end of the step are computed in [9] from the first and the third equation of (16). In [10], at last, the final values for the original variables x and $\dot{x}$ are computed for the end of the step, and we are ready for the next step.

20. The computational work in [3] and [10] of our flow chart is somewhat facilitated by the fact that certain of the time increments in our RUNGE-KUTTA formulas are equal, namely $t_1 - t_0 = t_4 - t_0 = h$. This means that the sums of [3] and [5] have to be computed three times only, and no new computation of the sums in [10] is necessary.
Furthermore, according to [2] and [3], $x_1 = x_4$. This means that for the computation of f_4 in [4] the part of f that depends on t and x but not on $\dot{x}$ could be taken over from the computation of f_1. In some cases--for instance equations (24) or (26)--this might practically reduce the number of evaluations of f by 1, as it does exactly in the case where f does not depend on $\dot{x}$ at all.

SECTION IV. THE EQUATIONS OF MOTION FOR THE RESTRICTED PROBLEM OF FOUR (THREE) BODIES

21. The restricted problem of four bodies is based on the following assumptions:

A. All four bodies (sun, earth, moon, space vehicle) are considered to be point masses that move in the same space-fixed plane.

B. The center of mass of the earth-moon system moves with constant angular velocity ω in a circle around the sun.

C. The earth and the moon move with constant angular velocity in circles around the center of mass of the earth-moon system.

D. The fourth body, the space vehicle, is of infinitesimal mass. Then, although attracted by the gravitational forces of the sun, the earth, and the moon, it can be considered to exert no gravitational forces on these bodies.

22. In the space-fixed plane (Figure 2) we consider two different coordinate systems:

A. The space-fixed ζ-system with the sun S as origin ($\zeta = \xi + i\eta$).

B. The body-fixed z-system with the center of mass C of the earth-moon system as the origin and the direction from the earth to the moon as the x-direction ($z = x+iy$).

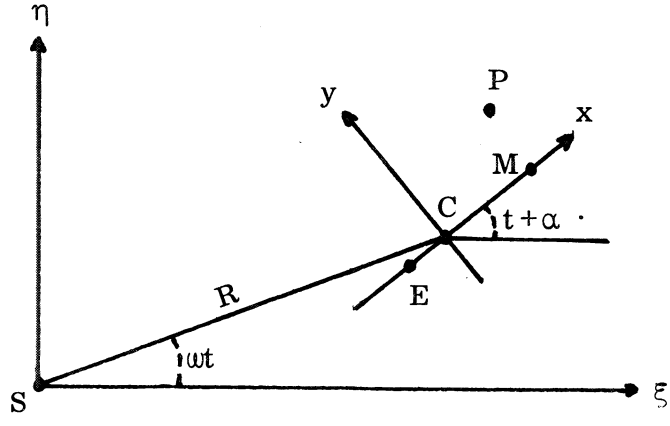

FIGURE 2. SPACE-FIXED PLANE

As is customary in the restricted problem of three bodies, we choose the mass of the earth-moon system as the mass unit, the distance from the earth E to the moon M as the unit of distance, and the time unit in such a way as to make the angular velocity of the earth-moon system around its center of mass C equal to 1. This implies that the gravitational constant in Newton's gravity law becomes equal to 1.

23. Let μ_S, $1-\mu$, μ, and m be the masses of the sun S, the earth E, the moon M, and the space vehicle P, respectively, and let 0, ζ_E, ζ_M, and ζ be their respective coordinates in the space-fixed ζ-system. To derive the equations of motion of the space vehicle we start from the Lagrangian function obtained for the space vehicle under the assumptions of the restricted problem of four bodies. Obviously, in the space-fixed ζ-system the Lagrangian function $L = T - U$ for the space vehicle reads as follows:

$$L = \frac{m}{2}|\dot{\zeta}|^2 + \frac{m(1-\mu)}{|\zeta - \zeta_E|} + \frac{m\mu}{|\zeta - \zeta_M|} + \frac{m\mu_S}{|\zeta|} \tag{18}$$

It is customary in the restricted problem of three bodies to study the motion of the space vehicle in the body-fixed rotating z-system. We shall use the same z-system for the restricted problem of four bodies. The following relations obviously hold between the coordinates in the ζ-system and the z-system:

$$\left.\begin{aligned} \zeta &= z\, e^{i(t+\alpha)} + Re^{i\omega t} \\ \zeta_E &= -\mu\, e^{i(t+\alpha)} + Re^{i\omega t} \\ \zeta_M &= (1-\mu)e^{i(t+\alpha)} + Re^{i\omega t} \end{aligned}\right\} \tag{19}$$

It follows from (19) that

$$|\zeta-\zeta_E| = |z+\mu|; \quad |\zeta-\zeta_M| = |z-(1-\mu)|; \quad |\zeta| = |z+Re^{i[(\omega-1)t-\alpha]}| \tag{20}$$

and by differentiation

$$\dot{\zeta} = (\dot{z}+iz)e^{i(t+\alpha)} + Ri\omega e^{i\omega t}$$

or

$$|\dot{\zeta}| = |(\dot{z}+iz) + i\omega Re^{i[(\omega-1)t-\alpha]}| \tag{21}$$

Introducing (20) and (21) into (18), we obtain for the Lagrangian function L in the body-fixed rotating z-system

$$L = \frac{m}{2}\left|(\dot{z}+iz) + i\omega Re^{i[(\omega-1)t-\alpha]}\right|^2 + \frac{m(1-\mu)}{|z+\mu|} + \frac{m\mu}{|z-(1-\mu)|} + \frac{m\mu_S}{|z+Re^{i[(\omega-1)t-\alpha]}|} \tag{22}$$

24. The equations of motion for the space vehicle in the case of the restricted problem of four bodies are then obtained from the Lagrangian equations of the second kind

$$\left.\begin{aligned} \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) - \frac{\partial L}{\partial x} &= 0 \\ \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{y}}\right) - \frac{\partial L}{\partial y} &= 0 \end{aligned}\right\} \tag{23}$$

by inserting expression (22) for L.

The insertion results in the following equations of motion for the space vehicle in the case of the restricted problem of four bodies, as can easily be verified:

$$\left.\begin{aligned} \ddot{x} &= 2\dot{y} + x + \omega^2 R\cos\varphi - \mu'\frac{x+\mu}{[(x+\mu)^2+y^2]^{3/2}} - \mu\frac{x-\mu'}{[(x-\mu')^2+y^2]^{3/2}} - \mu_S\frac{x+R\cos\varphi}{[(x+R\cos\varphi)^2+(y-R\sin\varphi)^2]^{3/2}} \\ \ddot{y} &= -2\dot{x} + y - \omega^2 R\sin\varphi - \mu'\frac{y}{[(x+\mu)^2+y^2]^{3/2}} - \mu\frac{y}{[(x-\mu')^2+y^2]^{3/2}} - \mu_S\frac{y-R\sin\varphi}{[(x+R\cos\varphi)^2+(y-R\sin\varphi)^2]^{3/2}} \end{aligned}\right\} \tag{24}$$

using the abbreviations

$$\mu' = 1 - \mu; \qquad \varphi = (1-\omega)t + \alpha \tag{25}$$

25. Omitting from (24) the terms contributed by the sun, our equations (24) reduce to the equations of motion for the space vehicle in the case of the restricted problem of three bodies:

$$\left.\begin{aligned} \ddot{x} &= 2\dot{y} + x - \mu'\frac{x+\mu}{[(x+\mu)^2+y^2]^{3/2}} - \mu\frac{x-\mu'}{[(x-\mu')^2+y^2]^{3/2}} \\ \ddot{y} &= -2\dot{x} + y - \mu'\frac{y}{[(x+\mu)^2+y^2]^{3/2}} - \mu\frac{y}{[(x-\mu')^2+y^2]^{3/2}} \end{aligned}\right\} \tag{26}$$

Equations (26) yield a first integral that can be obtained by multiplying the first equation in (26) by $\dot{x}$ and the second equation by $\dot{y}$, then adding both equations and integrating with respect to time t. The result is

$$\frac{1}{2}[(\dot{x}^2 + \dot{y}^2) - (x^2 + y^2)] - \frac{\mu'}{[(x+\mu)^2+y^2]^{1/2}} - \frac{\mu}{[(x-\mu')^2+y^2]^{1/2}} = \text{Const} = J \tag{27}$$

the so-called Jacobi integral.

SECTION V. THE RUNGE-KUTTA TRANSFORMATION METHOD APPLIED TO THE RESTRICTED PROBLEM OF FOUR (THREE) BODIES

26. Since we have explained our RUNGE-KUTTA transformation method in detail in Section III, we can now restrict ourselves to the problem of reducing the equations of motion (24) to an algebraic system of the second degree and deriving the recurrence formulas for the coefficients of the power series expansion for the solution of this second-degree system.

In a completely obvious and straightforward manner, we introduce the following eight auxiliary functions into (24):

$$\left.\begin{aligned} &\cos\varphi = a, \quad \sin\varphi = b \\ &(x+\mu)^2+y^2 = p^2, \quad (x-\mu')^2+y^2 = q^2, \quad (x+Ra)^2+(y-Rb)^2 = r^2 \\ &\frac{\mu'}{p^3} = u, \quad \frac{\mu}{q^3} = v, \quad \frac{\mu_S}{r^3} = w \end{aligned}\right\} \tag{28}$$

Including the equations and differential equations for these auxiliary functions, we obtain the following second-degree system instead of (24):

$$\left.\begin{aligned} \ddot{x} &= 2\dot{y}+x+\omega^2 Ra - u(x+\mu) - v(x-\mu') - w(x+Ra) \\ \ddot{y} &= -2\dot{x}+y-\omega^2 Rb - uy - vy - w(y-Rb) \\ \dot{a} &= -b(1-\omega) \\ \dot{b} &= a(1-\omega) \\ p^2 &= (x+\mu)^2+y^2 \\ q^2 &= (x-\mu')^2+y^2 \\ r^2 &= (x+Ra)^2+(y-Rb)^2 \\ p\dot{u}+3u\dot{p} &= 0 \\ q\dot{v}+3v\dot{q} &= 0 \\ r\dot{w}+3w\dot{r} &= 0 \end{aligned}\right\} \tag{29}$$

One might, at first glance, get discouraged when faced with ten equations. However, since system (29) is an algebraic system of the second degree, its numerical integration by power series expansions is completely trivial and is performed in exactly the same way as in the case of our simple example (1) in Section II.

27. Let us denote the coefficients of the power series expansion of the functions x, y, a, b, p, q, r, u, v, w by the capital letters X_ν, Y_ν, A_ν, B_ν, P_ν, Q_ν, R_ν, U_ν, V_ν, W_ν, respectively.
By introducing the power series expansions

$$x = \sum_{\nu=0} X_\nu (t-t_0)^\nu, \quad y = \sum_{\nu=0} Y_\nu (t-t_0)^\nu, \quad \ldots, \quad w = \sum_{\nu=0} W_\nu (t-t_0)^\nu$$

and their derivatives, if required, into (29) and comparing coefficients of equal powers--for instance, coefficients of $(t-t_0)^{n-1}$ or of $(t-t_0)^n$--one obtains in a completely straightforward way, the following recurrence formulas for the ten functions occurring in (29):

$$\left.\begin{aligned}
(n+1)nX_{n+1} &= 2nY_n + X_{n-1} + \omega^2 R A_{n-1} - \sum_{\nu=0}^{n-1} (U_\nu + V_\nu + W_\nu) X_{n-1-\nu} \\
&\quad - \mu U_{n-1} + \mu' V_{n-1} - R \sum_{\nu=0}^{n-1} W_\nu A_{n-1-\nu} \\
(n+1)nY_{n+1} &= -2nX_n + Y_{n-1} - \omega^2 R B_{n-1} - \sum_{\nu=0}^{n-1} (U_\nu + V_\nu + W_\nu) Y_{n-1-\nu} \\
&\quad + R \sum_{\nu=0}^{n-1} W_\nu B_{n-1-\nu} \\
nA_n &= -(1-\omega) B_{n-1}
\end{aligned}\right\} \qquad (30)$$

$$
\begin{aligned}
nB_n &= (1-\omega)A_{n-1} \\
2P_oP_n &= \sum_{\nu=0}^{n} X_\nu X_{n-\nu} + 2\mu X_n + \sum_{\nu=0}^{n} Y_\nu Y_{n-\nu} - \sum_{\nu=1}^{n-1} P_\nu P_{n-\nu} \\
2Q_oQ_n &= \sum_{\nu=0}^{n} X_\nu X_{n-\nu} - 2\mu' X_n + \sum_{\nu=0}^{n} Y_\nu Y_{n-\nu} - \sum_{\nu=1}^{n-1} Q_\nu Q_{n-\nu} \\
2R_oR_n &= \sum_{\nu=0}^{n} X_\nu X_{n-\nu} + 2R \sum_{\nu=0}^{n} X_\nu A_{n-\nu} + R^2 \sum_{\nu=0}^{n} A_\nu A_{n-\nu} \\
&\quad + \sum_{\nu=0}^{n} Y_\nu Y_{n-\nu} - 2R \sum_{\nu=0}^{n} Y_\nu B_{n-\nu} + R^2 \sum_{\nu=0}^{n} B_\nu B_{n-\nu} - \sum_{\nu=1}^{n-1} R_\nu R_{n-\nu} \\
nP_oU_n &= -3\sum_{\nu=1}^{n} \nu P_\nu U_{n-\nu} - \sum_{\nu=1}^{n-1} \nu U_\nu P_{n-\nu} \\
nQ_oV_n &= -3\sum_{\nu=1}^{n} \nu Q_\nu V_{n-\nu} - \sum_{\nu=1}^{n-1} \nu V_\nu Q_{n-\nu} \\
nR_oW_n &= -3\sum_{\nu=1}^{n} \nu R_\nu W_{n-\nu} - \sum_{\nu=1}^{n-1} \nu W_\nu R_{n-\nu}
\end{aligned}
\qquad (30) \text{ (continued)}
$$

For $n=1$, all sums in (30) with the lower limit $\nu=1$ and the upper limit $\nu = n-1$ have to be omitted.

When we start the computation for a certain step, we know, from the initial values for this step, the coefficients X_o, X_1 and Y_o, Y_1. From (28) we then obtain the coefficients A_o, B_o, P_o, Q_o, R_o, U_o, V_o, W_o. Setting $n = 1$, we find from (30) the coefficients X_2, Y_2, A_1, B_1, P_1, Q_1, R_1, U_1, V_1, W_1, and we continue by repeating the evaluation of the recurrence formulas (30) for $n = 2$, $n = 3$, etc. After having obtained in this way the coefficients X_2, X_3, ..., X_{m+2} and Y_2, Y_3, ..., Y_{m+2}, we are ready for our RUNGE-KUTTA transformation procedure as described in Section III.

In the case of the restricted problem of three bodies we start from equations (26) instead of equations (24). Equations (28) reduce, in this case, to four equations only. In a quite obvious way, (29) then reduces to six second-degree equations, and (30) reduces to six recurrence formulas.

SECTION VI. SOME NUMERICAL RESULTS FOR THE RESTRICTED PROBLEM OF THREE (AND FOUR) BODIES

28. In this section we present some of the numerical results we have obtained by applying the power series method (Section II) and our two RUNGE-KUTTA transformation methods (Section III) to the computation of a periodic orbit of the restricted problem of three bodies, and to the computation of the corresponding orbit--with the same initial conditions--for the restricted problem of four bodies.

29. Figure 3 shows, for the case of the restricted problem of three bodies, this periodic orbit in the rotating coordinate system.

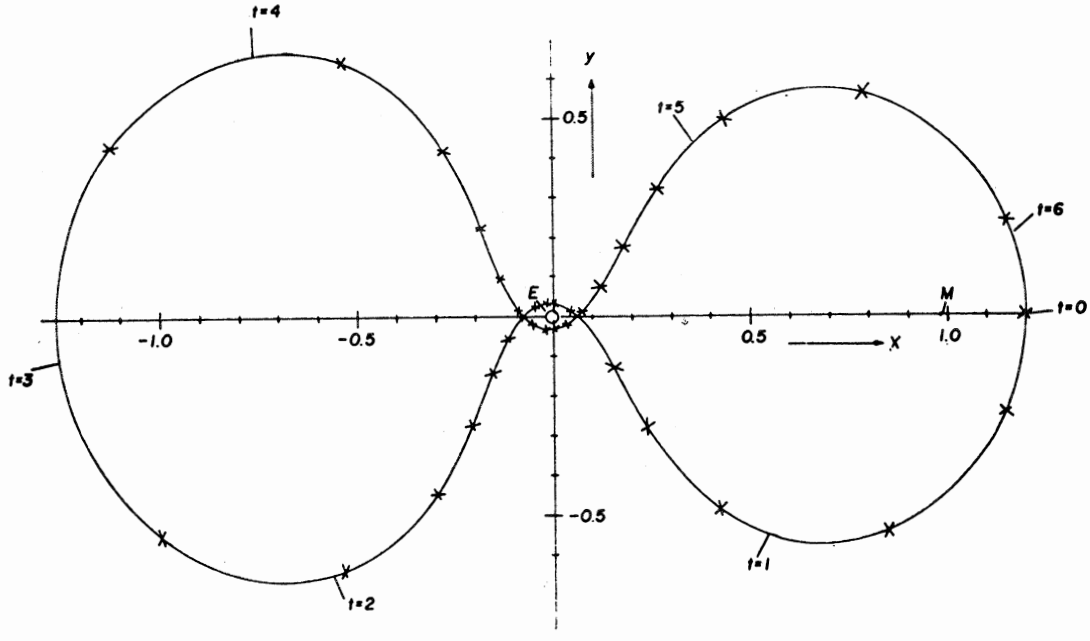

FIGURE 3. PERIODIC ORBIT IN THE ROTATING COORDINATE SYSTEM

The periodic orbit was used in previous papers by the author and has the following initial values:

$$x_0 = 1.2, \quad \dot{x}_0 = 0, \quad y_0 = 0, \quad \dot{y}_0 = -1.04935\,75098\,30320 \quad \left(\mu = \frac{1}{82.45}\right) \tag{31}$$

The initial value $\dot{y}_0$ in (31) was obtained by an interpolation procedure that varied $\dot{y}_0$ iteratively until the orbit, after half a period, finally crossed the x-axis perpendicularly. To preserve sufficient accuracy, the computation of $\dot{y}_0$ for the periodic orbit was performed in 20-digit arithmetic.

The computations presented in all tables in this paper were executed on an IBM 7094 digital computer (16 digits).

Tables I and II list the results that we have obtained, in the case of the restricted problem of three bodies, by the methods described in Sections II and III for one orbit (about one month actual time), and for 12 consecutive orbits (about one year actual time), starting from the initial values (31). The program came to an automatic stop when the orbit intersected the x-axis again after one or 12 complete orbits, respectively. The last point of intersection with the x-axis was obtained by continuously halving the step size for the last step until we missed the x-axis by less than a pre-set tolerance (10^{-17}).

Table I refers to eighth-order formulas (m = 4) and Table II to twelfth-order formulas (m = 8).

TABLE I. RESTRICTED PROBLEM OF THREE BODIES, RESULTS FOR EIGHTH-ORDER FORMULAS

Method*	No. of Orbits	Final x	Final $\dot{y}$	No. of Steps	Computer Running Time (min)
PSE	1	1.20000 00000 00040	-1.04935 75098 30345	1594	0.35
RKT 1	1	1.20000 00000 00103	-1.04935 75098 30421	1120	0.24
RKT 2	1	1.20000 00000 00038	-1.04935 75098 30366	840	0.19
PSE	12	1.20000 00000 00031	-1.04935 75098 30440	19134	4.20
RKT 1	12	1.20000 00000 00430	-1.04935 75098 31333	13459	2.78
RKT 2	12	1.20000 00000 00010	-1.04935 75098 30525	10080	2.11

(See footnote at end of Table II.)

TABLE II. RESTRICTED PROBLEM OF THREE BODIES, RESULTS FOR TWELFTH-ORDER FORMULAS

Method*	No. of Orbits	Final x	Final ẏ	No. of Steps	Computer Running Time (min)
PSE	1	1.19999 99999 99981	-1.04935 75098 30303	493	0.21
RKT 1	1	1.20000 00000 00001	-1.04935 75098 30321	389	0.15
RKT 2	1	1.20000 00000 00013	-1.04935 75098 30332	290	0.13
PSE	12	1.20000 00000 00071	-1.04935 75098 30531	5896	2.49
RKT 1	12	1.19999 99999 99991	-1.04935 75098 30373	4740	1.83
RKT 2	12	1.20000 00000 00097	-1.04935 75098 30627	3353	1.35

* { PSE = Power Series Expansion Method [10]
RKT 1 = Runge-Kutta Transformation Method [11]
RKT 2 = Runge-Kutta Transformation Method [12]

All methods listed in Tables I and II were run with automatic step-size control for every step. The step size was accepted if for this step size Δt--but not for double the step size $2 \cdot \Delta t$--the absolute value of the truncation errors T_x and T_y in x and y were smaller than $|x_0| \cdot 10^{-16}$, $|y_0| \cdot 10^{-16}$, respectively, with x_0 and y_0 standing for the initial values for x and y for the current step. Comparing the computer running time in both tables, it becomes evident that twelfth-order formulas require considerably less computer time than eighth-order formulas--not to mention the prohibitively slow fourth-order standard RUNGE-KUTTA formulas. In fact, our twelfth-order formulas require only about 60 to 65 percent of the time for the eighth-order formulas. This time saving for the twelfth-order formulas is a consequence of the smaller number of steps required for a twelfth-order formula (only about 1/3 of the number required for an eighth-order formula in our example).

Moreover, Tables I and II show a significant time saving for our RUNGE-KUTTA transformation method compared with the power series expansion method. Our

more recently developed RUNGE-KUTTA transformation method (RKT 2) gives results of about the same accuracy as the power series expansion method (PSE) in about half the computer time.

As the x- and $\dot{y}$-values of the tables show, all three methods are of about the same accuracy for equal tolerances; after 12 orbits we lost, in all methods, about 2 to 3 digits in x and $\dot{y}$. This means that even after 12 orbits we miss the initial value x_0 of (31) by only about 1/100 millimeter actual distance--certainly a negligible deviation.

30. We now turn to the restricted problem of four bodies. For this problem we computed an orbit with the same initial conditions (31) that we used for our periodic orbit (Figure 3) in the case of the restricted problem of three bodies. The results of our computations, if compared with our previous computations, will give an indication of how the attractive force of the sun affects our orbit of Figure 3. Naturally, the periodicity of our orbit is lost if the influence of the sun is taken into account. However, the shape of our orbit remains approximately preserved for a surprisingly long time. Since the differential equations (24) for the restricted problem of four bodies are more involved than the corresponding differential equations (26) for the restricted problem of three bodies, the numerical integration of equations (24) naturally took longer on the computer--about twice as long as for equations (26).

In Tables III and IV we list our results for the restricted problem of four bodies. We use the starting values (31) and set $\alpha = 0$ in (25). These assumptions mean that sun, earth, moon, and space vehicle are initially all located on one straight line. We also made machine runs for other values for α. However, because these changes in the configuration of the bodies do not produce any essential changes in our results, we can restrict ourselves here to presenting only the case where $\alpha = 0$.

TABLE III. RESTRICTED PROBLEM OF FOUR BODIES, RESULTS FOR EIGHTH-ORDER FORMULAS

Method*	No. of Orbits	Final x	Final $\dot{y}$	No. of Steps	Computer Running Time (min)
PSE	1	1.19033 91358 54073	-1.02487 19211 55096	1578	0.67
RKT 1	1	1.19033 91358 54174	-1.02487 19211 55201	1117	0.58
RKT 2	1	1.19033 91358 54125	-1.02487 19211 55176	835	0.43
PSE	12	1.17279 62121 74518	-1.01782 10547 51673	18144	7.69
RKT 1	12	1.17279 62121 75284	-1.01782 10547 52938	12954	6.61
RKT 2	12	1.17279 62121 74671	-1.01782 10547 52064	9723	5.00

* See footnote at end of Table II.

TABLE IV. RESTRICTED PROBLEM OF FOUR BODIES, RESULTS FOR TWELFTH-ORDER FORMULAS

Method*	No. of Orbits	Final x	Final $\dot{y}$	No. of Steps	Computer Running Time (min)
PSE	1	1.19033 91358 54114	-1.02487 19211 55165	485	0.38
RKT 1	1	1.19033 91358 54016	-1.02487 19211 55062	401	0.34
RKT 2	1	1.19033 91358 54004	-1.02487 19211 55048	287	0.27
PSE	12	1.17279 62121 74782	-1.01782 10547 52114	5598	4.35
RKT 1	12	1.17279 62121 74791	-1.01782 10547 51654	5125	4.14
RKT 2	12	1.17279 62121 74737	-1.01782 10547 51634	3280	2.73

* See footnote at end of Table II.

In our machine programs we again applied exactly the same automatic step-size control procedure, including the same tolerances, and the same procedure for the last (closing) step as in the case of the restricted problem of three bodies.

Since, in the case of the restricted problem of four bodies, the numerically correct values for our problem are not known, we can try to determine the accuracy of our methods only by comparing the results for the different methods. Lacking a better criterion for accuracy, it seems reasonable to assume that those digits in the final values for x and $\dot{y}$ which are in agreement for all methods are correct. But again, then, we do not lose more than 3 digits even after 12 orbits. This means, again, that the deviations in x among the different methods and the true solutions are, after 12 orbits, still of the order of 1/100 millimeter. With respect to saving computer time--whether using twelfth-order formulas instead of eighth-order formulas or using our RUNGE-KUTTA transformation method instead of the power series method--we obtained about the same results as for the case of the restricted problem of three bodies.

31. The orbit that we have considered is not perturbed very much by the influence of the sun, at least not for the first year for which we have run our computations. The deviations in x from $x_0 = 1.2$ to $x = 1.17279...$ after 12 orbits correspond to a deviation of about 10,460 kilometers, which is less than one earth diameter. We also determined the x-deviations for the 1st, 2nd, 3rd, ..., 11th orbit; they never exceed one earth diameter and seem to have an oscillatory behavior. However, periodic orbits of the restricted problem of three bodies which come closer to the moon than does our orbit turn out to be more sensitive to the influence of the sun and the moon. For such orbits, our model of the restricted problem of four bodies might no longer be sufficiently realistic. One might have to include the ellipticity of the moon orbit to obtain a satisfactory approximation of the real conditions. But, since this paper is mainly concerned with numerical integration procedures, we did not proceed further in the direction of a more realistic model.

The methods described in this paper are, however, applicable to considerably more involved problems than the restricted problem of three (or four) bodies. Actually, these methods have been applied in our Computation Laboratory to the problem of N oblate bodies as well as to the problem of the powered flight of a space vehicle--in both cases with rather favorable results.

George C. Marshall Space Flight Center
National Aeronautics and Space Administration
Huntsville, Alabama, June 1, 1966

APPENDICES

32. In Appendices A through C we present summaries of some other numerical integration methods that we found interesting or promising and that are applicable to problems such as we have described in Section IV. Since these methods were developed and published by other authors, we restrict ourselves to presenting short descriptions without any derivation of the formulas. However, we shall give sufficient references to the original papers.

In these appendices we also present, for comparison, some numerical results obtained for these methods, applied to the problems of Section IV. We have tried to give an unbiased review of the methods in question, but it should be understood that we have based our opinion of these methods on their practical applicability to problems in celestial mechanics, such as we have described in Section IV.

APPENDIX A

HIGH-ORDER EXPLICIT RUNGE-KUTTA FORMULAS

33. In this appendix we consider the explicit RUNGE-KUTTA formulas of E. B. SHANKS [18], [19]. These formulas represent a remarkable extension of the traditional 4-th-order RUNGE-KUTTA formulas to higher-order formulas. Naturally, the number of evaluations per step of the differential equations increases with the order of the formulas. However, the increase is not so sharp as to make high-order formulas uneconomical for an electronic computer. On the contrary, since higher-order formulas permit--without loss of accuracy--a larger step size than 4-th-order formulas, the differential equations can be integrated in considerably fewer steps. This more than compensates for the increased computational effort per step in such high-order formulas.

34. The most interesting and highest-order formula of E. B. SHANKS is an 8-th-order formula based on 12 evaluations of the differential equations. We restrict ourselves to quoting this 8-th-order formula and applying it to the problems of Section IV.

E. B. SHANKS' 8-th-order formula reads, when written in the traditional notation:

$$
\begin{aligned}
k_1 &= f(t_0, x_0)h \\
k_2 &= f\left(t_0 + \frac{1}{9}h, x_0 + \frac{1}{9}k_1\right)h \\
k_3 &= f\left(t_0 + \frac{1}{6}h, x_0 + \frac{1}{24}k_1 + \frac{1}{8}k_2\right)h \\
k_4 &= f\left(t_0 + \frac{1}{4}h, x_0 + \frac{1}{16}k_1 + \frac{3}{16}k_3\right)h \\
k_5 &= f\left(t_0 + \frac{1}{10}h, x_0 + \frac{29}{500}k_1 + \frac{33}{500}k_3 - \frac{3}{125}k_4\right)h \\
k_6 &= f\left(t_0 + \frac{1}{6}h, x_0 + \frac{11}{324}k_1 + \frac{1}{243}k_4 + \frac{125}{972}k_5\right)h \\
k_7 &= f\left(t_0 + \frac{1}{2}h, x_0 - \frac{7}{12}k_1 + \frac{19}{9}k_4 + \frac{125}{36}k_5 - \frac{9}{2}k_6\right)h \\
k_8 &= f\left(t_0 + \frac{2}{3}h, x_0 - \frac{10}{81}k_1 - \frac{32}{243}k_4 + \frac{125}{243}k_5 + \frac{11}{27}k_7\right)h \\
k_9 &= f\left(t_0 + \frac{1}{3}h, x_0 + \frac{1175}{324}k_1 - \frac{32}{3}k_4 - \frac{3125}{162}k_5 + 26k_6 + \frac{121}{162}k_7 - \frac{1}{12}k_8\right)h \\
k_{10} &= f\left(t_0 + \frac{5}{6}h, x_0 + \frac{293}{324}k_1 - \frac{71}{27}k_4 - \frac{1375}{324}k_5 + \frac{51}{9}k_6 - \frac{59}{162}k_7 + \frac{1}{2}k_8 + k_9\right)h \\
k_{11} &= f\left(t_0 + \frac{5}{6}h, x_0 + \frac{1303}{1620}k_1 - \frac{71}{27}k_4 - \frac{1375}{324}k_5 + \frac{37}{6}k_6 + \frac{103}{162}k_7 + \frac{1}{10}k_{10}\right)h \\
k_{12} &= f\left(t_0 + h, x_0 - \frac{955}{492}k_1 + \frac{2560}{369}k_4 + \frac{8125}{738}k_5 - \frac{612}{41}k_6 + \frac{7}{82}k_7\right. \\
&\quad \left. - \frac{27}{164}k_8 - \frac{18}{41}k_9 - \frac{12}{41}k_{10} + \frac{30}{41}k_{11}\right)h \\
x &= x_0 + \frac{1}{840}(41k_1 + 216k_6 + 272k_7 + 27k_8 + 27k_9 + 36k_{10} + 180k_{11} + 41k_{12}) + 0(h^9)
\end{aligned}
\qquad \text{(A-1)}
$$

35. We have programmed SHANKS' formulas (A-1) for the restricted problem of three--as well as four--bodies. Since no better step-size control procedure seems to exist for SHANKS' formulas, we have applied RICHARDSON's deferred approach to the limit. This, naturally, is a considerable additional

computational effort merely for the benefit of step-size control.

We have run the orbits of Section VI with SHANKS' formulas (A-1) on the same electronic computer and with the same tolerance 10^{-16} that we used for the various methods for which we listed numerical results in Section VI. The following Tables, A-I and A-II, present the results of the runs we made with SHANKS' formulas for one orbit.

TABLE A-I. RESTRICTED PROBLEM OF THREE BODIES

Method	No. of Orbits	Final x	Final $\dot{y}$	No. of Steps	Computer Running Time (min)
RKS*	1	1.20000 00000 00002	-1.04935 75098 30310	814	0.46

TABLE A-II. RESTRICTED PROBLEM OF FOUR BODIES

Method	No. of Orbits	Final x	Final $\dot{y}$	No. of Steps	Computer Running Time (min)
RKS*	1	1.19033 91358 54033	-1.02487 19211 55064	817	1.63

* RKS = RUNGE-KUTTA-SHANKS (8-th-order formula)

The accuracy of SHANKS' formulas (A-1) is quite impressive. Comparison of the final values in Table A-I with the initial values (31) shows that we lose only 1 digit in x and 2 digits in $\dot{y}$. This is somewhat less than we lose in Table I for the power series expansion method and our RUNGE-KUTTA transformation methods when set up as 8-th-order methods. The running time for SHANKS' formulas, however, is considerably longer than for the methods of Tables I and III. In the restricted problem of three bodies SHANKS' method takes about twice as long as our RKT 2 method, and in the restricted problem

of four bodies almost four times as long. The numerous evaluations--required by SHANKS' method--of the trigonometric functions sin φ and cos φ, occurring in equations (24), account for the relatively long running time for this method in the case of the restricted problem of four bodies. The presence of transcendental functions in the differential equations will always slow SHANKS' method, since in his 8-th-order formula these functions have to be evaluated 23 times per step (including step-size control procedure) versus 4 evaluations per step for our RUNGE-KUTTA transformation formulas.

Naturally, in our methods in Sections II and III we must also pay for the computation of the derivatives that are required in these methods. However, the computation (especially of the lower-order derivatives) is rather easy and fast by the use of our recurrence formulas.

SHANKS' formulas might gain considerably if a less expensive but still reliable step-size control procedure were available for them.

However, since SHANKS' formulas are of 8-th order at best, one cannot expect them to compete with our higher-order formulas, as a comparison of Tables A-I and A-II with the first part of Tables II and IV clearly indicates.

APPENDIX B

HIGH-ORDER IMPLICIT RUNGE-KUTTA FORMULAS

36. In explicit RUNGE-KUTTA formulas--for instance, Formula (A-1)--the computation of the increment k_ν requires a knowledge of only the preceding increments $k_1, k_2, \ldots k_{\nu-1}$. Therefore, in explicit RUNGE-KUTTA formulas, all increments k_ν can be computed one after the other in one procedure.
In implicit RUNGE-KUTTA formulas the increment k_ν depends not only on the preceding increments $k_1, k_2, \ldots k_{\nu-1}$ but also on k_ν itself and on the succeeding increments $k_{\nu+1}, k_{\nu+2}, \ldots$. Therefore, in implicit RUNGE-KUTTA formulas, the increments k_ν have to be determined by an iterative procedure. Naturally, such an iterative computation is more involved than the straightforward procedure for explicit RUNGE-KUTTA formulas.
However, there are some points in favor of implicit RUNGE-KUTTA formulas. For instance, implicit RUNGE-KUTTA formulas are available for any order, whereas no explicit RUNGE-KUTTA formulas exceeding the 8-th order are known so far.

37. Implicit RUNGE-KUTTA formulas have been studied by J. KUNTZMANN and his collaborators. We mention as a reference the textbook of F. CESCHINO and J. KUNTZMANN [9]. More recently, J. C. BUTCHER has published two noteworthy papers on implicit RUNGE-KUTTA methods. In these papers he derived various implicit formulas based on the quadrature formula of GAUSS-LEGENDRE [4] or on quadrature formulas of RADAU [5]. The latter formulas have the advantage of requiring fewer iterative k_ν stages than the formulas based on the GAUSS-LEGENDRE quadrature formula. In a

separate paper [7], J. C. BUTCHER presents 20-digit tables for the coefficients of his implicit RUNGE-KUTTA formulas (up to the 20-th order).

38. Let us illustrate the procedure for implicit RUNGE-KUTTA formulas by quoting one of BUTCHER's 8-th-order formulas based on RADAU's quadrature formulas:

$$
\left.
\begin{aligned}
k_1 &= f(x_0)h \\
k_2 &= f(x_0 + \beta_{21}k_1 + \beta_{22}k_2 + \beta_{23}k_3 + \beta_{24}k_4)h \\
k_3 &= f(x_0 + \beta_{31}k_1 + \beta_{32}k_2 + \beta_{33}k_3 + \beta_{34}k_4)h \\
k_4 &= f(x_0 + \beta_{41}k_1 + \beta_{42}k_2 + \beta_{43}k_3 + \beta_{44}k_4)h \\
k_5 &= f(x_0 + \beta_{51}k_1 + \beta_{52}k_2 + \beta_{53}k_3 + \beta_{54}k_4)h \\
\\
x &= x_0 + C_1k_1 + C_2k_2 + C_3k_3 + C_4k_4 + C_5k_5 + 0(h^9)
\end{aligned}
\right\} \quad \text{(B-1)}
$$

It is assumed that the independent variable t does not appear explicitly on the right-hand side of the differential equation. This is no restriction, however, since by the introduction of an additional dependent variable (which is identical with t) the independent variable t can always be eliminated on the right-hand side of the differential equation.

From (B-1) it follows that these implicit RUNGE-KUTTA formulas, which correspond to SHANKS' formulas (A-1), have only three iterative stages (k_2, k_3, k_4) and only five stages altogether.

Formulas of 12-th-order of the type (B-1) would contain five iterative stages and seven stages altogether.

In (B-1) one first computes k_1 and starts the iteration for k_2, k_3, k_4 by introducing into the right-hand side of the 2nd, 3rd, and 4th equation the value k_1 as the first approximation of k_2, k_3, k_4. After the iteration procedure has converged to the final values k_2, k_3, k_4, the last two equations of (B-1) yield k_5 and the x-value for the end of the step.

J. C. BUTCHER has pointed out that a step-size control procedure is possible for formulas of the type (B-1) by combining these formulas with implicit RUNGE-KUTTA formulas of the same order but based on the GAUSS-LEGENDRE quadrature formula. This means, however, that the computational effort has to be doubled to obtain a reliable step-size control. In this respect, one is faced with the same situation as in the case of explicit RUNGE-KUTTA formulas.

39. Using BUTCHER's formulas of the type (B-1), and for step-size control the corresponding formulas of the GAUSS-LEGENDRE type, we again computed the orbit of Section VI for the restricted problem of three bodies. Table B-I presents the results of the runs we made with BUTCHER's 8-th- and 12-th-order formulas.

TABLE B-I. RESTRICTED PROBLEM OF THREE BODIES

Method	No. of Orbits	Final x	Final $\dot{y}$	No. of Steps	Computer Running Time (min)
RKB (8)*	1	1.20000 00000 00010	-1.04935 75098 30318	870	1.56
RKB (12)*	1	1.20000 00000 00013	-1.04935 75098 30328	216	0.88

* { RKB (8) = RUNGE-KUTTA-BUTCHER (8-th-order formula)
RKB (12) = RUNGE-KUTTA-BUTCHER (12-th-order formula)

The runs were made on the same computer and with the same tolerances for the truncation error as the runs reported in Section VI and in Appendix A. The values in Table B-I can be compared with the first half of Tables I, II, and A-I. Quite obviously, in our example, the implicit RUNGE-KUTTA formulas are much slower than the corresponding explicit RUNGE-KUTTA formulas or the RUNGE-KUTTA transformation formulas.

However, since implicit RUNGE-KUTTA formulas are available for any order of accuracy, they might be rather attractive for some problems which require high-order accuracy.

APPENDIX C

MODIFIED MULTISTEP METHODS

40. Although this paper deals with one-step methods, for comparison we shall consider in this appendix the new modified multistep formulas suggested by J. C. BUTCHER [8]. We have already mentioned in Section I that these new formulas are much more convenient than the traditional multistep formulas since they are based on fewer backward steps than were the earlier formulas.

For instance, BUTCHER's 7-th-order formula is based on only three equidistant backward points t_n, t_{n-1}, t_{n-2}, whereas the traditional 7-th-order implicit multistep formula of ADAMS requires six equidistant backward points t_n, t_{n-1}, t_{n-2}, t_{n-3}, t_{n-4}, t_{n-5}.

As already pointed out in Section I, the stability restrictions of the traditional multistep methods are overcome in the case of the modified multistep methods by the introduction of one additional non-step point. This requires one additional formula for the non-step point. But this additional computational effort seems more than compensated for by the convenience of the new formulas. Since they are based on fewer backward points, the starting procedure and the change of interval size is much more easily performed for these formulas than for the traditional multistep formulas.

41. BUTCHER's multistep formulas are of the predictor-corrector type consisting of two predictor formulas for the non-step point and for the next step point, and one corrector formula for the next step point. The formulas require three evaluations of the differential equations per step. In his paper [8], BUTCHER presents such multistep formulas of the 5-th, 7-th, 9-th, 11-th, and 13-th order.

For instance, let us consider his 7-th-order formulas. For a first-order differential equation $\dot{x} = u(t, x)$ his formulas read:

$$\left.\begin{aligned}
\hat{x}_{n+1/2} &= x_n - \frac{25}{16}(x_n - x_{n-1}) - \frac{153}{128}(x_n - x_{n-2}) \\
&\quad + h\left(\frac{225}{128}u_n + \frac{75}{32}u_{n-1} + \frac{45}{128}u_{n-2}\right) + 0(h^6) \\
\hat{x}_{n+1} &= x_n + \frac{297}{31}(x_n - x_{n-1}) + \frac{212}{21}(x_n - x_{n-2}) \\
&\quad + h\left(\frac{384}{155}\hat{u}_{n+1/2} - 9\,u_n - \frac{426}{31}u_{n-1} - \frac{309}{155}u_{n-2}\right) + 0(h^6) \\
x_{n+1} &= x_n + \frac{135}{617}(x_n - x_{n-1}) + \frac{31}{617}(x_n - x_{n-2}) \\
&\quad + h\left(\frac{93}{617}\hat{u}_{n+1} + \frac{2304}{3085}\hat{u}_{n+1/2} - \frac{27}{617}u_n - \frac{99}{617}u_{n-1} - \frac{39}{3085}u_{n-2}\right) + 0(h^8)
\end{aligned}\right\} \quad \text{(C-1)}$$

The subscript $n+1/2$ denotes the non-step auxiliary point that is required for stability reasons.

These formulas (C-1) were also used in an iterative way when starting the method and when halving the integration step size.

In the latter case, we proceeded from the 5-th-order formula

$$\left.\begin{aligned}
x_{n-1/2} &= \frac{45}{128}x_n + \frac{9}{16}x_{n-1} + \frac{11}{128}x_{n-2} \\
&\quad + h\left(-\frac{9}{128}u_n + \frac{9}{32}u_{n-1} + \frac{3}{128}u_{n-2}\right) + 0(h^6)
\end{aligned}\right\} \quad \text{(C-2)}$$

as a first approximation for the half-step point.

In the case of a second-order differential equation $\ddot{x} = f(t, x, u)$, a convenient approximation for the leading term of the truncation error for x_{n-1} in (C-1) reads:

$$
\left.
\begin{aligned}
T_{x_{n+1}} = h\Big(&\frac{93}{617}\hat{u}_{n+1} + \frac{2304}{3085}\hat{u}_{n+1/2} - \frac{463}{1234}u_{n+1} \\
&- \frac{459}{1234}u_n - \frac{171}{1234}u_{n-1} - \frac{73}{6170}u_{n-2}\Big) \\
&+ h^2\Big(\frac{51}{1234}f_{n+1} - \frac{351}{1234}f_n - \frac{81}{1234}f_{n-1} - \frac{3}{1234}f_{n-2}\Big)
\end{aligned}
\right\} \qquad \text{(C-3)}
$$

The formula (C-3) is obtained by constructing an 8-th-order formula for x_{n+1} which coincides with the third formula in (C-1), as far as the x-terms are concerned

$$
\left.
\begin{aligned}
x_{n+1} = x_n &+ \frac{135}{617}(x_n - x_{n-1}) + \frac{31}{617}(x_n - x_{n-2}) \\
&+ h\Big(\frac{463}{1234}u_{n+1} + \frac{405}{1234}u_n - \frac{27}{1234}u_{n-1} - \frac{1}{1234}u_{n-2}\Big) \\
&+ h^2\Big(-\frac{51}{1234}f_{n+1} + \frac{351}{1234}f_n + \frac{81}{1234}f_{n-1} + \frac{3}{1234}f_{n-2}\Big) + 0(h^9)
\end{aligned}
\right\} \qquad \text{(C-4)}
$$

and subtracting (C-4) from the third equation of (C-1).

42. We have applied BUTCHER's 7-th-order formulas to the restricted problem of three bodies. The point of intersection with the x-axis of our periodic orbit (Figure 3) after a complete period was found from the coordinates, velocities, and accelerations for the last three points of the orbit by Hermitian interpolation.

While all results in Section VI and in Appendices A and B were obtained using an error tolerance of 10^{-16}, we had to relax the tolerance somewhat in the case of BUTCHER's multistep method. In view of the magnitude of some of the coefficients of the predictor formulas, the necessity for such a relaxation is not surprising. We ran BUTCHER's formulas for an error tolerance of $5 \cdot 10^{-16}$ and of 10^{-15}.

TABLE C-I. RESTRICTED PROBLEM OF THREE BODIES

Results for 7-th-Order Formulas
Tolerance: $5 \cdot 10^{-16}$

Method	Final x	Final $\dot{y}$	No. of Steps	Computer Running Time (min)
BUTCHER	1.19999 99999 99904	-1.04935 75098 31055	3370	0.63
PSE	1.20000 00000 01013	-1.04935 75098 31284	2118	0.38
RKT 2	1.20000 00000 00124	-1.04935 75098 30410	1097	0.20

TABLE C-II. RESTRICTED PROBLEM OF THREE BODIES

Results for 7-th-Order Formulas
Tolerance: 10^{-15}

Method	Final x	Final $\dot{y}$	No. of Steps	Computer Running Time (min)
BUTCHER	1.20000 00000 01204	-1.04935 75098 31504	2799	0.53
PSE	1.20000 00000 02329	-1.04935 75098 32640	1913	0.35
RKT 2	1.20000 00000 00239	-1.04935 75098 30579	989	0.18

Tables C-I and C-II show the results of the runs we made for BUTCHER's modified multistep formulas and for certain other methods described in this report, always comparing methods of the same order and runs with the same error tolerance.

Since a multistep method is based on a number of backward steps, it necessarily has a larger truncation error than a one-step method. A multistep method therefore requires a larger number of steps for our orbit.

In Tables C-I and C-II the computer running times are rather closely proportional to the number of steps, independently of the individual method.

For BUTCHER's multistep method this means that, although this method requires only three evaluations of the differential equations per step, it is not faster per step than the one-step methods we have considered. Obviously, much of the speed of the multistep method is lost by the frequent step size changes required in our problem. Any halving of the step size requires an expensive (forward and backward) iteration procedure to maintain sufficient accuracy. Therefore, multistep methods are not well-suited to problems that require frequent changes in the integration step size. Under the circumstances it is still somewhat surprising how well BUTCHER's multistep method is doing in our example compared with the one-step methods listed.

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